Electronic Spectra of Benzene: An APCELL Experiment[1]

Joe Shapter[1] and Jason Gascooke[2]

[1]School of Chemistry, Physics and Earth Science, Flinders University, Sturt Road, Bedford Park, South Australia, 5042, joe.shapter@flinders.edu.au. [2]Department of Chemistry, University of Adelaide, South Australia, 5005

Spectroscopy is a cornerstone of modern chemistry. It is of course a window to the quantum nature of atoms and molecules. The quantum structure of matter is introduced very early and covered in some depth in most educational programs. The hands-on application of spectroscopy to probe energy levels is the ideal way to crystallise for students the quantum structure of atoms and molecules.

This experiment was developed to expose students to both the energetic structure of a molecule (the electronic structure of benzene in this case) and to the "mechanics" of spectroscopy. The electronic structure of benzene is probed through the collection of both absorption and excitation spectra in the ultraviolet regain. The spectra obtained are not the same and hence the student must think about how and why peaks are obtained in a given spectrum and then must use this understanding to explain the observed difference. While the different forms of spectroscopy (absorption vs. emission for example) are often discussed in lectures, students rarely get to do a hands-on comparison of the differences in the lab. This is a particularly nice example as the method of data collection affects the result. Assignment of the spectra gives the students an understanding of the quantum levels under interrogation.

The absorption part of the experiment was originally taken from " The Theory and Applications of Ultraviolet Spectroscopy", H. H. Jaffé and M. Orchin, Wiley (1962) pp. 134 –144. The laser part of the experiment was developed in its entirety at Flinders with the help of several undergraduate students.

Educational Template

Section 1 - Summary of the Experiment

1.1 Experiment Title

Electronic Spectra of Benzene

1.2 Description of the Experiment

All the building blocks of nature, atoms and molecules, are quantum mechanical in their nature. This means they have well defined energy states in which they can exist and they cannot exist with energy in between these states. It is possible to change the system from one state to another by either adding energy to make a "jump" from a lower level to a higher one (assuming the added energy is exactly the amount of the gap) or allowing the system to "fall" from a high energy state to a lower one. This second process happens spontaneously in many cases and is used for example in Neon lights.

In this experiment, students are exposed to many rules about the transitions between states in both the "up" and "down" direction. This practical will help students understand how those transitions occur and further will demonstrate in a very obvious way that what goes up does NOT necessarily come back down—at least not the same way.

The "up" transitions are measured using standard UV spectrometer to measure an absorption spectrum of benzene. The "down" transitions are probed using a N_2 laser set up where benzene is excited to an upper state and then allowed to fall back down. The fluorescence which results from these transitions is measured. Comparisons of the two spectra show the differences in transitions in the two directions.

1.3 Course Context and Students' Required Knowledge and Skills

The basic understanding of the quantum mechanical nature of systems is generally covered in most Physical Chemistry textbooks and will be undertaken by most students in second or perhaps first year at university. The description of the lab further reinforces these ideas if the students lack some of the background. The practical also illustrates the different magnitudes of some of the transitions possible (electronic versus vibrational).

Quantum mechanical transitions are responsible for many everyday events. The most obvious examples involve the production of light for example in neon signs and lasers such as the diode laser used in CD players.

A knowledge of the quantum mechanical nature of matter is useful in this practical. The lab skills required are very common for most undergraduate students for the absorption part of the experiment. All modern instruments will be computer driven and the operational is quite simple. The laser part of the experiment can be more complicated and students will need a basic introduction to the system but then should be able to collect the data independently.

1.4 Time Required to Complete

Prior to Lab	1 hour
In Laboratory	12 hours
After Laboratory	2 hours

1.5 Other Comments

This experiment is one of the few examples of the use of a research grade piece of equipment in an undergraduate lab. Also, there are very few examples of the comparison of excitation and deactivation processes in undergraduate labs.

The two separate experiments outlined in this practical can be done as separate experiments but the learning outcomes would need to be adjusted as the comparison knowledge that comes with it would be lost.

Section 2 – Educational Analysis

Theoretical and Conceptual Knowledge:
Students are presented from a very early stage the concept of the quantum nature of atoms and molecules. One of the most obvious ways to confirm the "model" is through spectroscopy where students can "see" transitions between the various levels in the atoms or molecules. This experiment reinforces these ideas by first allowing the student to collect spectra themselves and hence watch it being collected so they see rises and falls in intensity. Of course, at the end of the collection the overall spectrum reinforces the idea that only certain transitions are possible and hence matter must be quantised.

The second idea presented in the prac is the notion that light can both be adsorbed by molecules or emitted (if the molecule is first excited). Students do both experiments and in fact are shown quite dramatically that the two processes are not always identical.

Scientific and Practical Skills:
Scientific skills include the operation of a laser and an uv-vis spectrometer. The second of these is really quite straightforward but the first requires considerable hands on work by the students in for example, tuning doubling crystals and scanning dye lasers. Analysis of the spectrum forces the students to "convert" their observations into a model of the energy states of the system. Finally, normalising is necessary as emission spectra collected over different wavelength regions have different intensities. Using the overlapping region, one spectrum of normalised intensity can be determined.

Practical skills involved include presentation of very specific scientific data in a particular and meaningful way. The understanding of much of the instrumentation is more of a scientific skill in this case given the nature of the equipment.

Generic Skills:
Generic skills from this prac do include (but are not limited to) all the skills that many current day experiments insist on: computer collection and presentation of data, report writing, spreadsheet manipulation and presentation of data (in a special way as outlined earlier), communication of the results.

This experiment does present a somewhat unique opportunity for students to develop some other generic skills. For one of the few times, students, in essence, collect the same data twice using two different methods. The uniqueness here possibly lies in the fact that the results are dramatically different. This forces the student into a problem solving situation involving the critical analysis of their data (is it right?) and the ability to apply their well-grounded knowledge to explain an unexpected result. This will help the development of skills that are at the root of life-long learning.

Learning Outcomes *What will students learn?*	**Process** *How will students learn it?*	**Assessment** *How will staff know students have learnt it?* *How will students know they have learnt it?*
Theoretical and Conceptual Knowledge		
Quantum nature of atoms/ molecules	Record and EXPLAIN spectra	Correct assignment of peaks Understanding of peak separation will reinforce quantum nature of matter
Light can be absorbed	Record uv-vis spectrum and explain the observation of various intensities (peaks)	Be able to run instrument and get spectrum. Produce a diagram of the transitions involved in absorption.
Light can be emitted	Record the emission spectrum using laser excitation. Explain the transitions (both up and down) involved	Using the relatively complicated system, the students can watch the spectrum as it is collected. Using the diagram from the point above, show the transitions involved in the laser part of the experiment.
Scientific and Practical Skills		
Use of the equipment is summarised in 2 and 3 above		
Measurements of Absorption Spectra.	Record uv-vis spectrum	Check of spectrum

[1]The complete documentation for this experiment is freely available on the APCELL web site [www.apcell.org]. It includes the educational template, a set of student notes, demonstrator notes and technical notes to allow ready implementation into a new laboratory.

Normalising Spectra	Student will have to overlay two spectra with appropriate scaling	Check of the final overall spectra Students can add together spectra with various weighting to see what differences occur.
Presentation of complex data	As above and in final report	Report assessment and feedback
Generic Skills		
Computer use	Used to collect and process data at every stage as well as present final findings	Monitoring of experimental use in addition to assessment of spectra and final reports.
Writing/Communication Skills	During the experiment, students explain the transitions observed verbally. In produce a report, the student must write a detailed account of a highly technical, complicated experiment and provide lucid explanations of observations.	Discussion during the lab will focus on assignment of the transitions to ensure the student has the proper understanding of the peak assignments and can express those understandings. Report marking will show if the student can, in writing, provide understandable detailed explanations.
Explanation of new observation	Explaining the difference in recorded spectra	Quality of explanation and the demonstration of the difference between absorption and emission.

Section 3 – Student Learning Experience

3.1 Did this experiment help you to understand the theory and concepts of the topic? If so, how, or if not, why not?

S1: Yes. It linked two concepts (fluorescence and absorbance) and explained their relationship. It was also good in that it linked this prac with both a previous prac, and the lectures.

S2: Yes, I always find it helpful in understanding theory when I can see it occurring in front of me and I know the conditions under which the observations have been made.

3.2 How is this experiment relevant to you in terms of your interests and goals?

S1: Anybody who wants to become a physical chemist needs to have some understanding about how molecules behave and this prac clearly teaches you something about this.

S2: I enjoy seeing theory that I am learning or have learnt being put into practice. This experiment assisted me in grasping the theory and giving me greater confidence for the exam. It also made me more confident in retaining the knowledge as it was no longer simply a set of rules or theories to remember but could be applied to results I could visualise and explain myself.

3.3 Did you find this experiment interesting? If so, what aspects of this experiment did you find of interesting? If not, why not?

S1: Yes. It was a good introduction to lasers.

S2: Yes. The opportunity to use a sophisticated piece of machinery and to be able to operate it myself as well as transferring the data and being able to manipulate it to produce a meaningful graph that could be related to the theory.

3.4 Can the experiment be completed comfortably in the allocated time? Is there time to reflect on the tasks while performing them?

S1: Yes and Yes (while waiting for results).

S2: Yes, there was plenty of time to complete the prac and enough time to apply the theory myself. There was also ample time to consult the demonstrator and even to fool around with the equipment a little to become more comfortable with it.

3.5 Does this experiment require teamwork and if so, in what way? Was this aspect of the experiment beneficial?

S1: No, it was a one-on-one situation between student and demonstrator

S2: This experiment did not really require any teamwork although comparison with others who had done the prac to assess the reproducibility of the results can be done.

3.6 Did you have the opportunity to take responsibility for your own learning, and to be active as learners?

S1: Yes, the prac involved questions that needed to be thought about between prac sessions and while writing the report.

S2: Once the basic methods of operation were demonstrated, I was left with a series of steps to work through, using my knowledge of the apparatus to confirm what was expected from the basic theory. There was time both during the prac and before the next session to consult textbooks and lecture notes about the relevant theory.

3.7 Does this experiment provide for the possibility of a range of student abilities and interests? If so, how?

S1: Yes, mainly because there was a demonstrator solely to help you so if you needed to ask a lot of questions you had the opportunity to do so.

S2: Yes, because the actual operation of the apparatus is not difficult, the theory can be discussed with the demonstrator in greater detail if necessary.

3.8 Did the laboratory notes, demonstrator's guidance and any other resources help you in learning from this experiment? If so, how?

S1: The demonstrator's guidance definitely helped as he was there to help throughout the whole prac, showing me how to use the equipment and asking me questions to make me keep thinking (but also giving hints when needed).

S2: The laboratory notes assisted in jogging my memory of the basic theory and operation of the apparatus while the demonstrator was helpful when I encountered mechanical problems (due to the trial nature of the prac rather than intrinsic problems of the apparatus) and also in asking questions to lead me towards greater understanding of the theory.

3.9 Are there any other features of this experiment that made it a particularly good or bad learning experience for you?

S1: The way the prac linked other work (another prac and the lectures) and ideas was great.

S2: It was a good learning experience in learning to work independently and gaining greater confidence with unfamiliar apparatus.

3.10 What improvements could be made to this experiment?

S1: Perhaps a little info to read before you enter the lab would be useful (it was very new when I did it though, so obviously there hadn't been much time to organise that yet)

S2: None.

3.11 Any Other Comments

[no responses]

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With all the initiatives being developed and implemented by chemists, as I have indicated above and which was very obvious to those at the meeting, there is a need to evaluate the effectiveness of these initiatives in a rigorous manner. This is far from an easy task and educational research approaches are often needed that are too time-consuming for busy chemists. Here is an opportunity for collaboration between chemistry educators with an orientation towards the development of enhanced chemistry experiences for students and chemistry educators with an orientation towards the evaluation of these experiences. As was illustrated by a series of papers on 'Representations in chemistry and their effect on learning', I believe that several of us at Curtin University and the University of Western Australia are progressing in this direction. By the next RACI Chemical Education Division meeting in Hobart in February 2004 we look forward to sharing more of that research work on the evaluation of learning outcomes from different teaching/learning approaches.

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An invitation

The editors invite readers to make contributions to this Journal. As well as papers submitted for peer review, we welcome any of the following:

- **Short papers on chemistry topics or concepts, from an educational perspective**
- **Reflective papers teaching and learning chemistry - general or specific**
- **Letters to the editor**
- **Announcements**
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- **Forthcoming events**
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